Alanine, 2-methyl-

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 187 °C

Global applicability domain: Inside

Local applicability domain index: 2.69e-01

Confidence level: 7.83e-01

Nearest Neighbors from the Training Set

Image not found

Pentanoic acid
Measured: 186
Predicted: 181

Image not found

2-Methylbutanoic acid
Measured: 177
Predicted: 177

Image not found

Isovaleric acid
Measured: 177
Predicted: 177

Image not found

Ethoxyacetic acid
Measured: 207
Predicted: 195